Electronic Supplementary Information

A Cascade Oxidation/[4+1] Annulation of Sulfonium Salts for Synthesis of Polyfunctional Furans: DMSO as One-Carbon Source

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Electronic Supplementary Information

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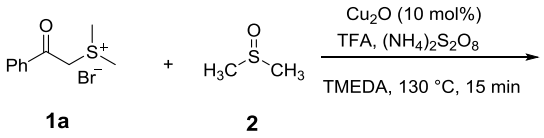
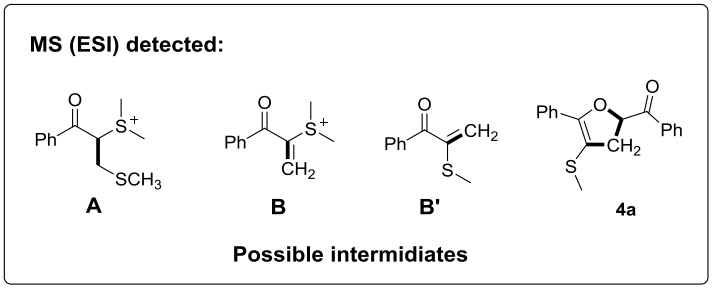
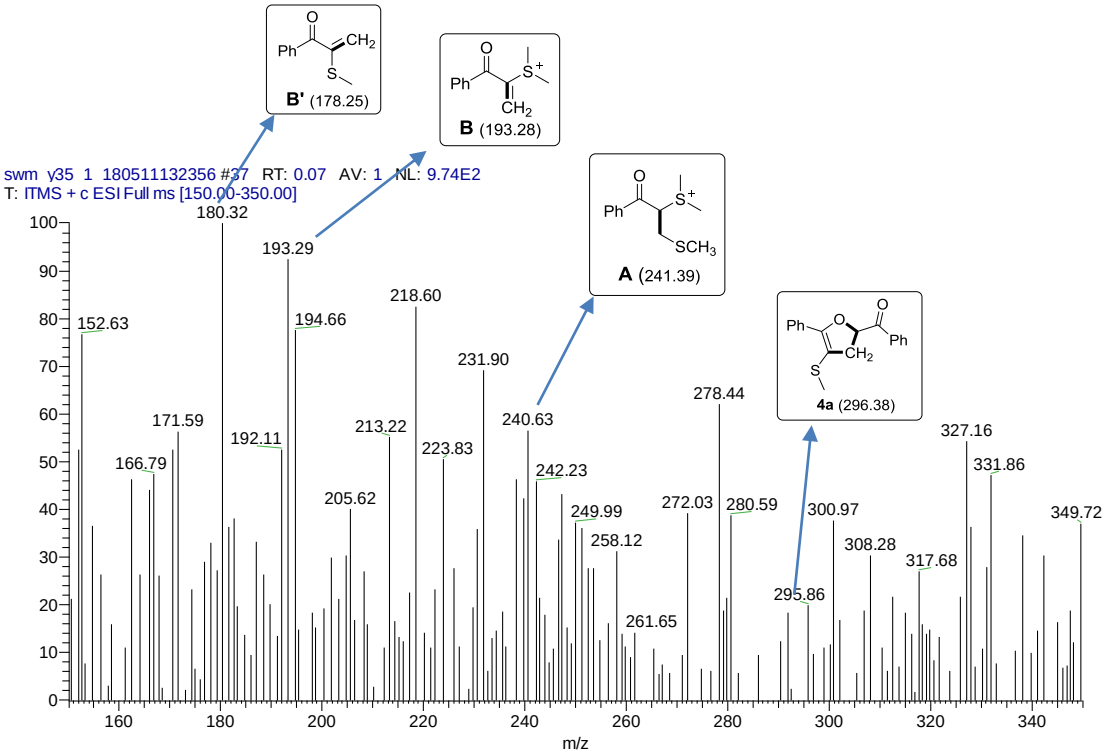
The following intermediates were detected.



1a 2





2. The Crystallographic Data

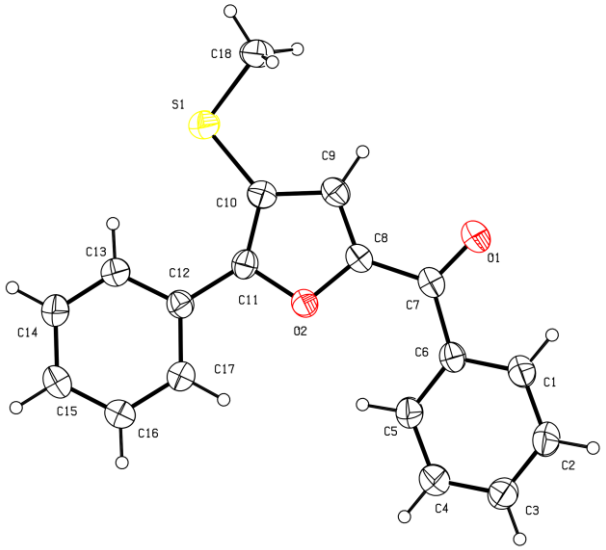
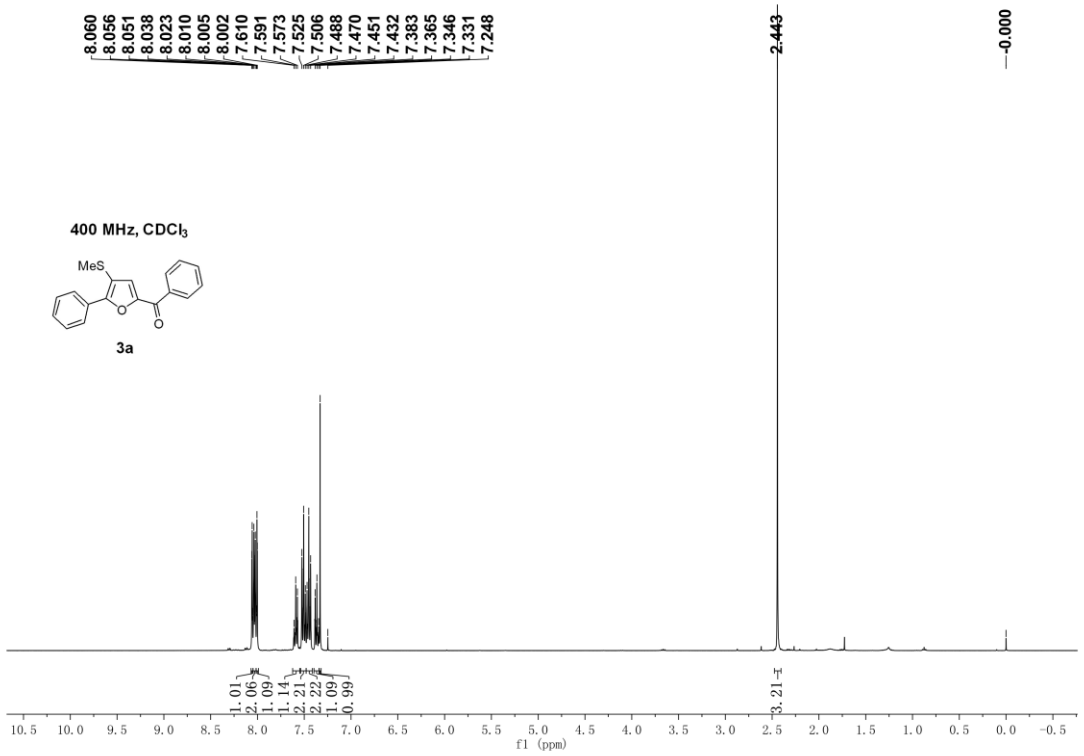
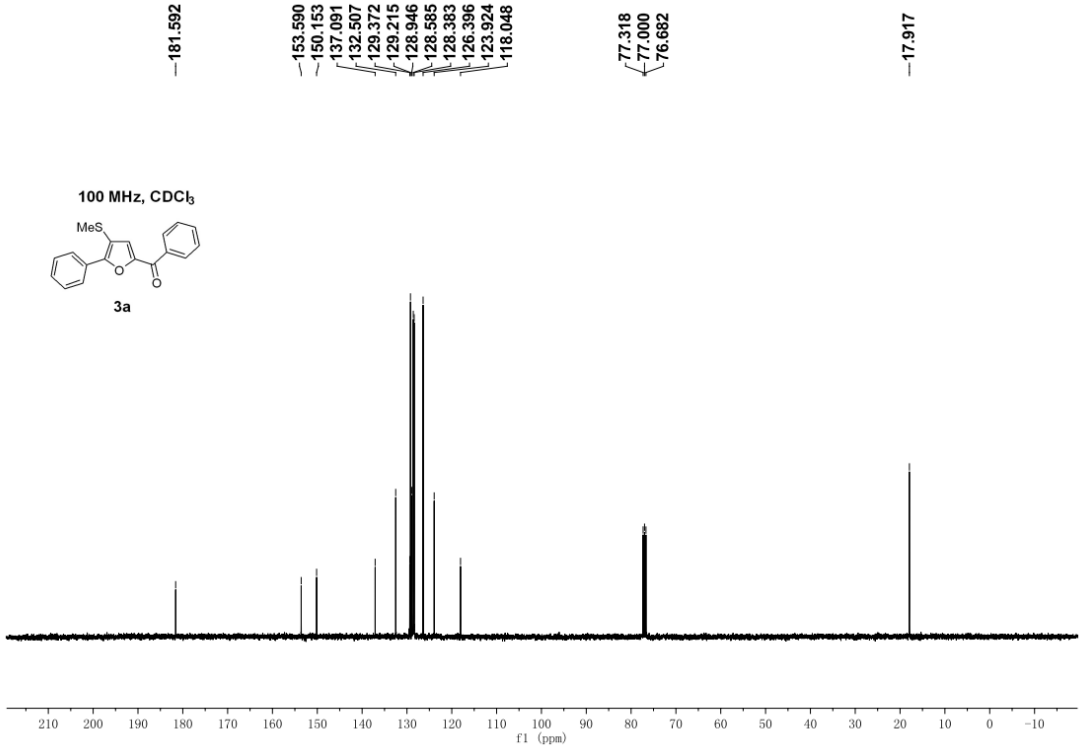


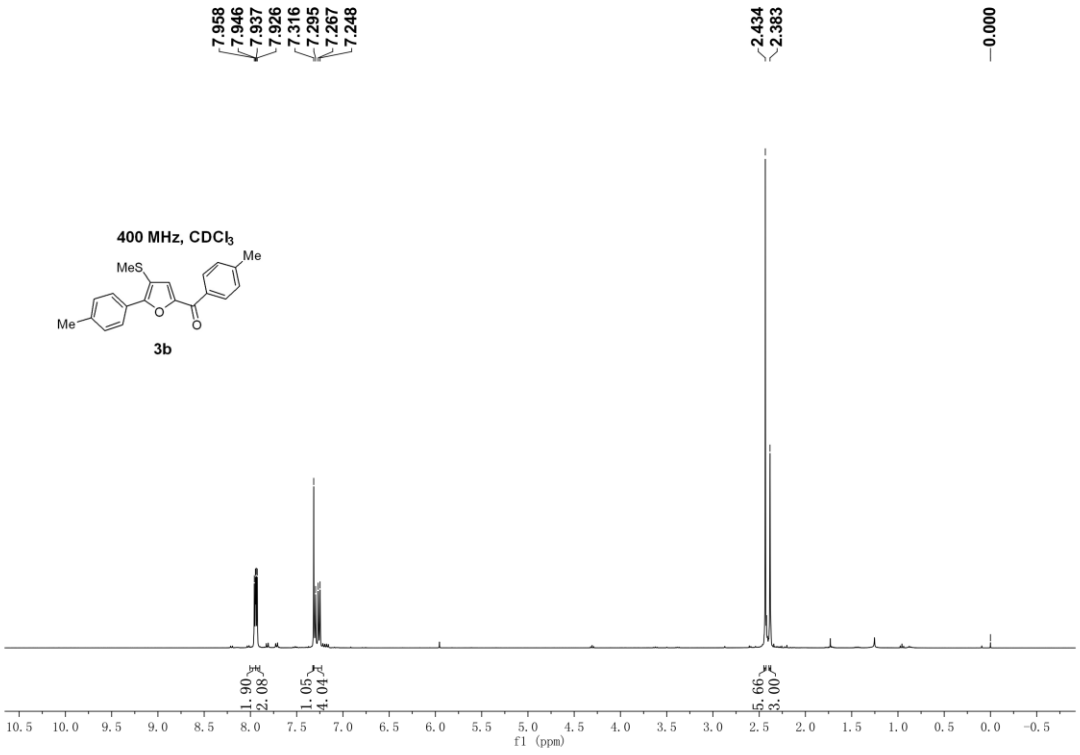
Table S1. The crystallographic data of **3a** (CCDC: 1848092).

Empirical formula	$C_{18}H_{14}O_2S$	
Formula weight	294.35	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.270(3) Å	a= 90 °.
	b = 5.3525(11) Å	b= 103.956(4) °.
	c = 20.691(4) Å	g = 90 °.
Volume	1426.3(5) Å3	
Z	4	
Density (calculated)	1.371 Mg/m^3	
Absorption coefficient	0.228 mm^{-1}	
F(000)	616	
Crystal size	0.220 x 0.200 x 0.180 mm^3	
Theta range for data collection	1.581 to 26.510 °.	
Reflections collected	10661	
Independent reflections	2943 [R(int) = 0.0498]	
Completeness to theta = 25.242 °	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2943 / 0 / 191	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1332	
R indices (all data)	R1 = 0.0854, wR2 = 0.1574	
Largest diff. peak and hole	0.194 and -0.233 e.$Å^{-3}$	

3. Appendix: spectral copies of ^{1}HNMR, and ^{13}CNMR



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7.295
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7.248
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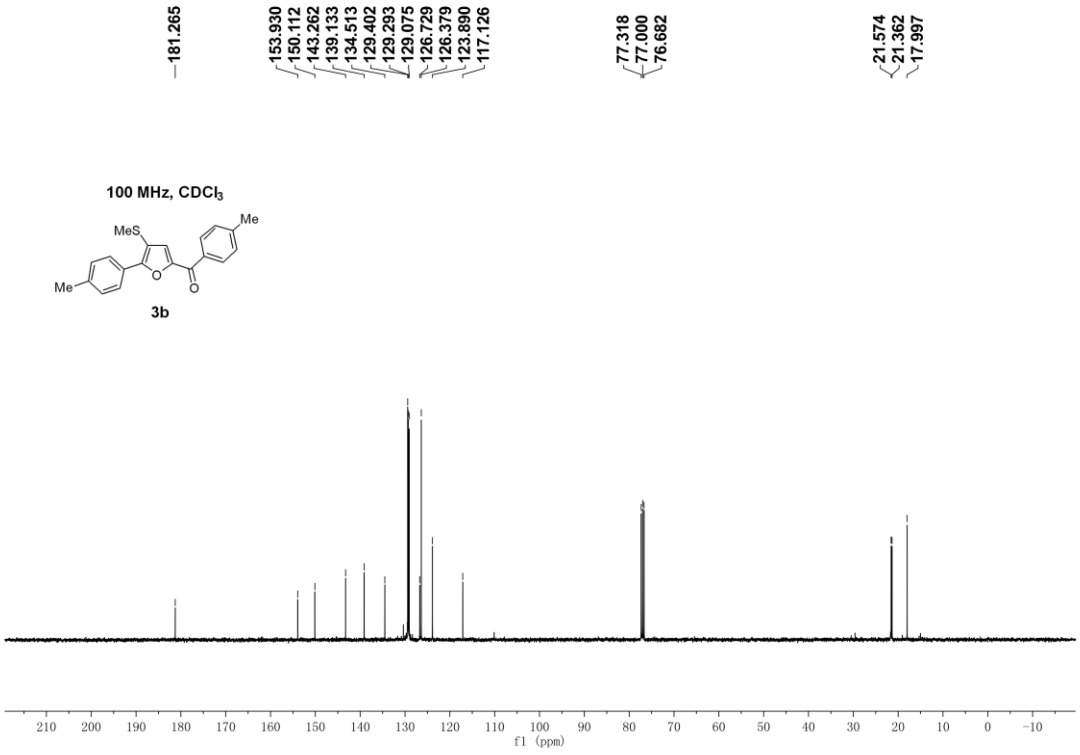
MeS
Me
Me
O
O
3b
1.90
2.08
1.05
4.04
5.66
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.000
76.682
21.574
21.362
17.997
100 MHz, CDCl3
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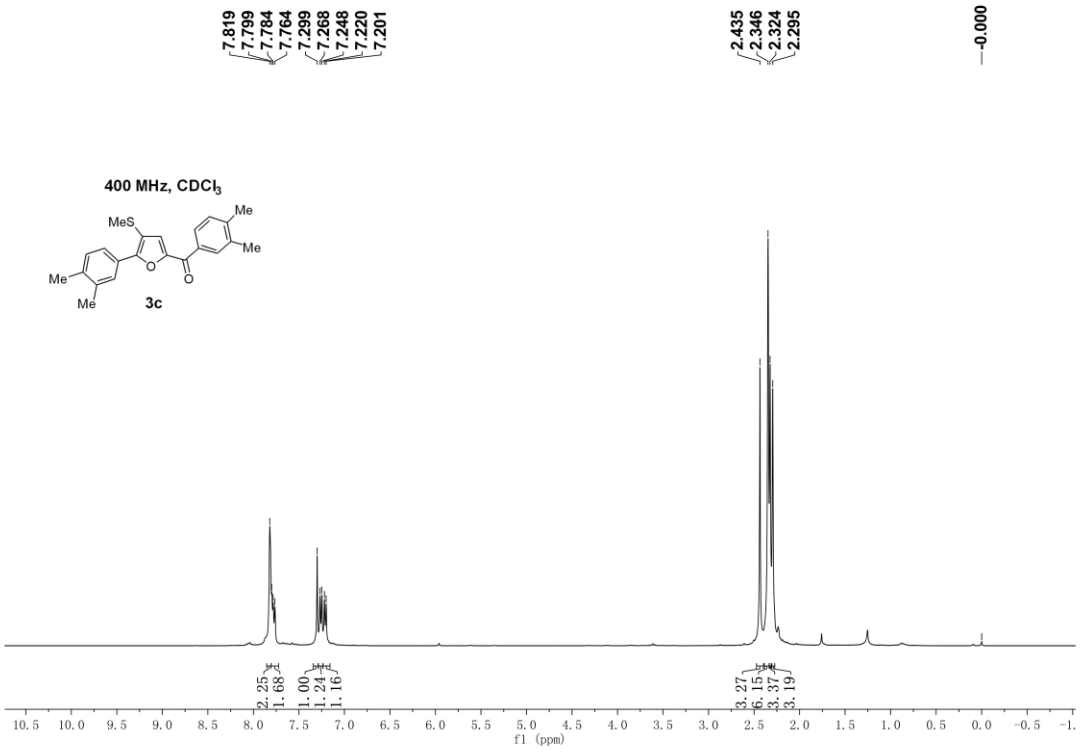
Me
Me
O
O
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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2.295
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Me
Me
Me
Me
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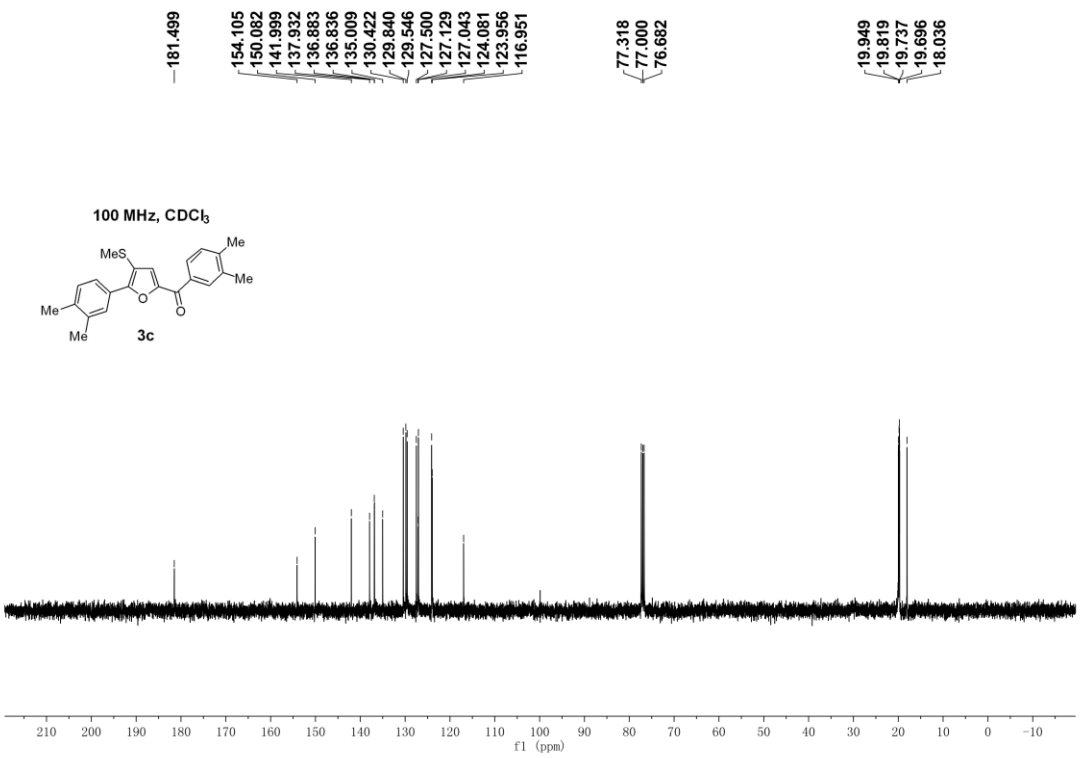
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127.129
127.043
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123.956
116.951
77.318
77.000
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19.949
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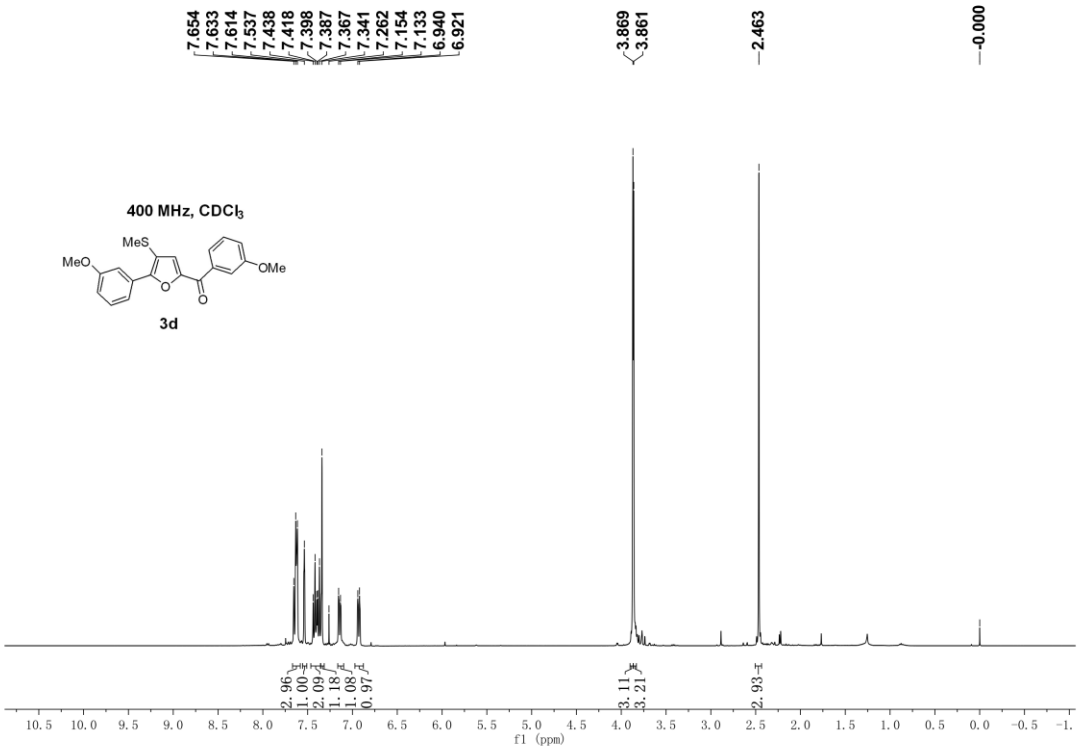
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MeO
OMe
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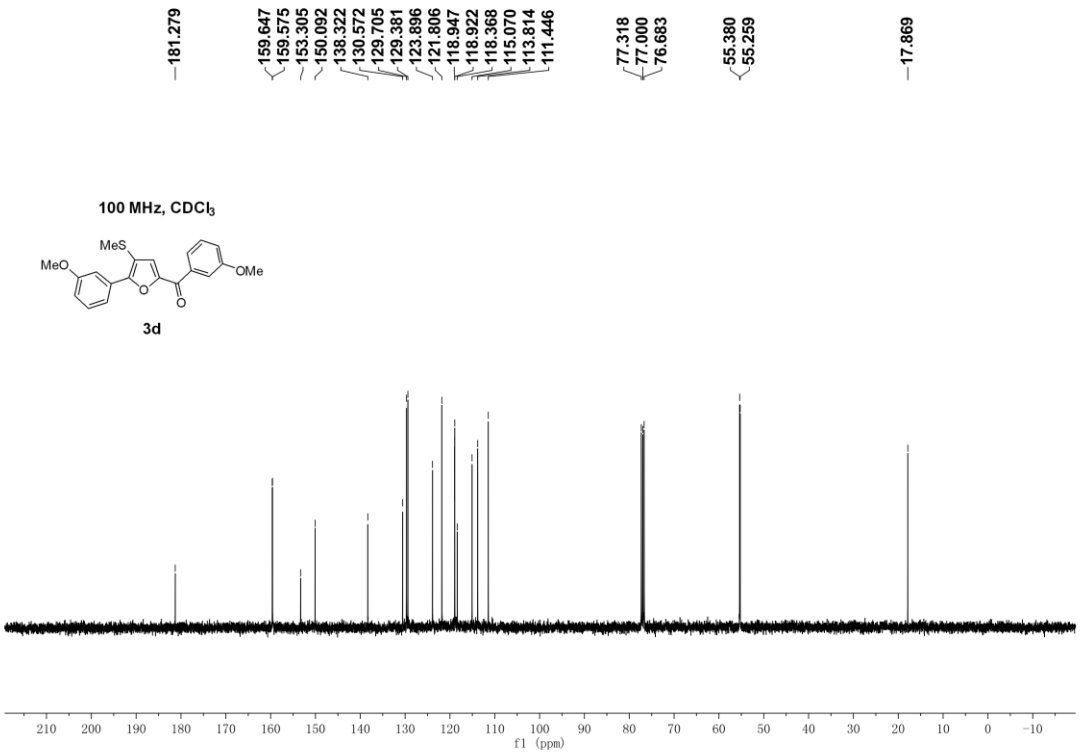
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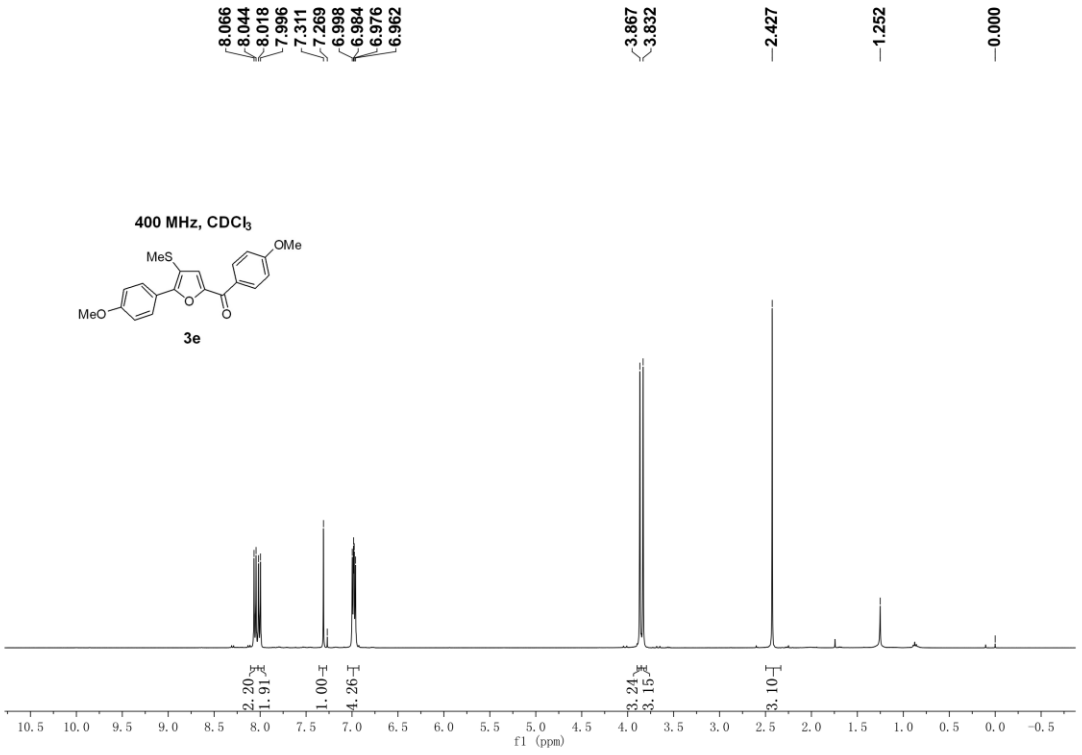
MeO
OMe
O
3d
f1 (ppm)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400 MHz, CDCl3
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OMe
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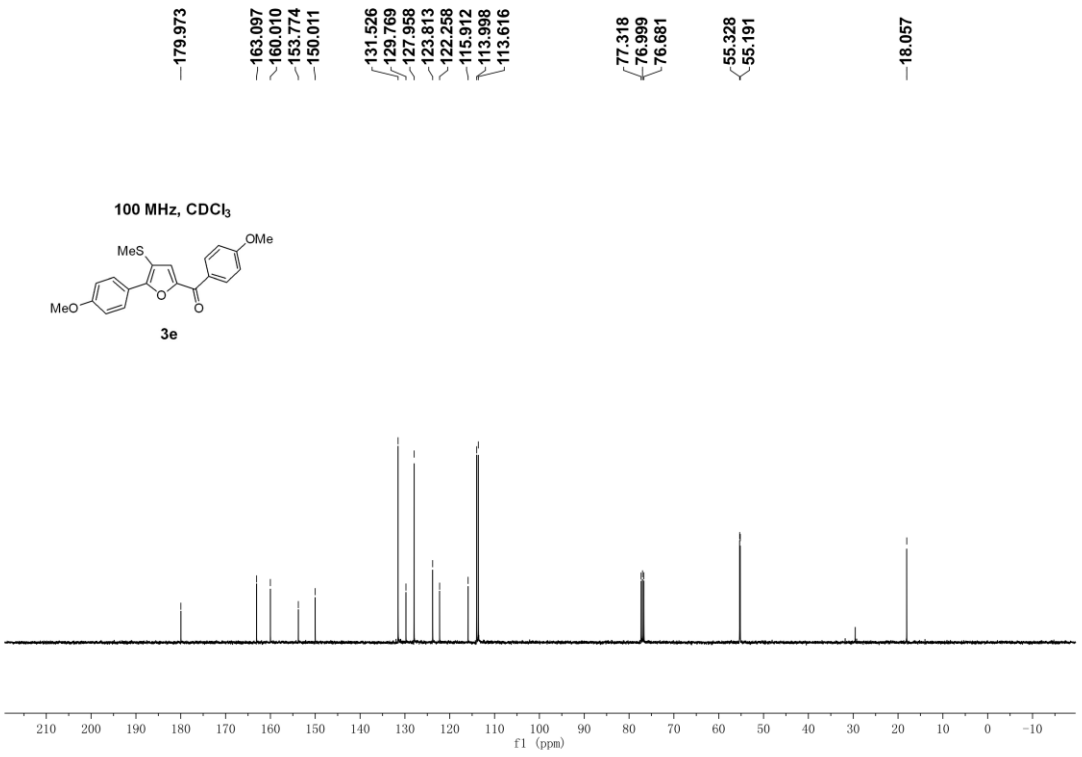
f1 (ppm)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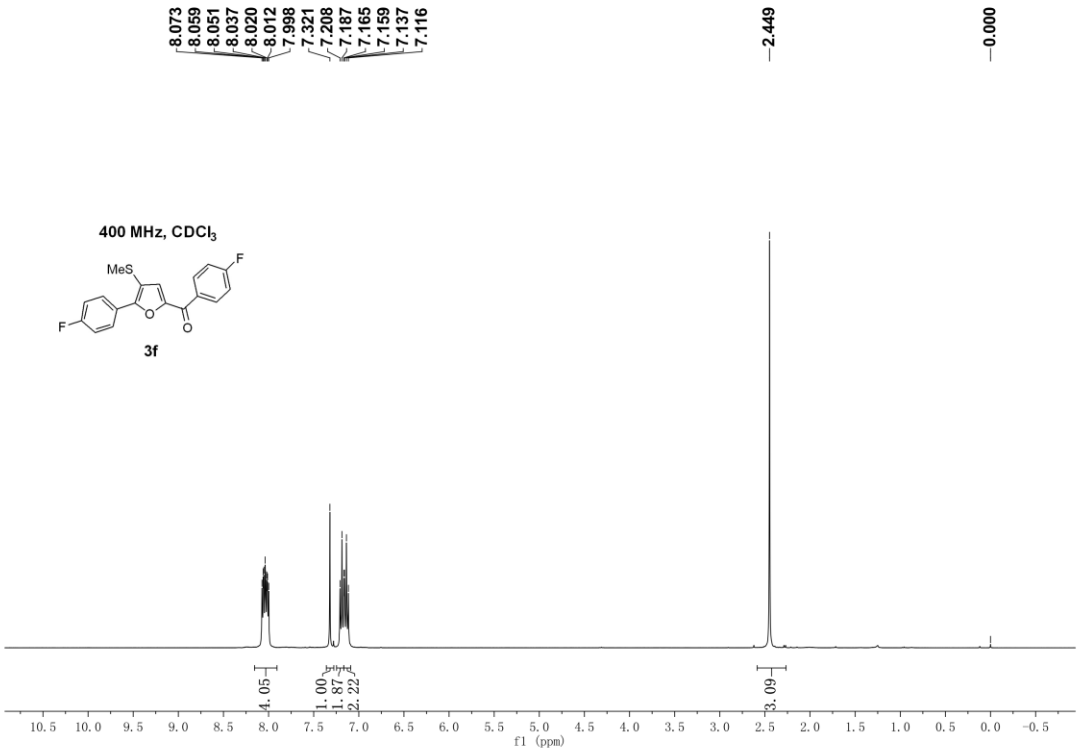
MeO
O
3e
f1 (ppm)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7.116
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0.000
400 MHz, CDCl3
MeS
F
F
O
3f
4.05
1.00
1.87
2.22
3.09
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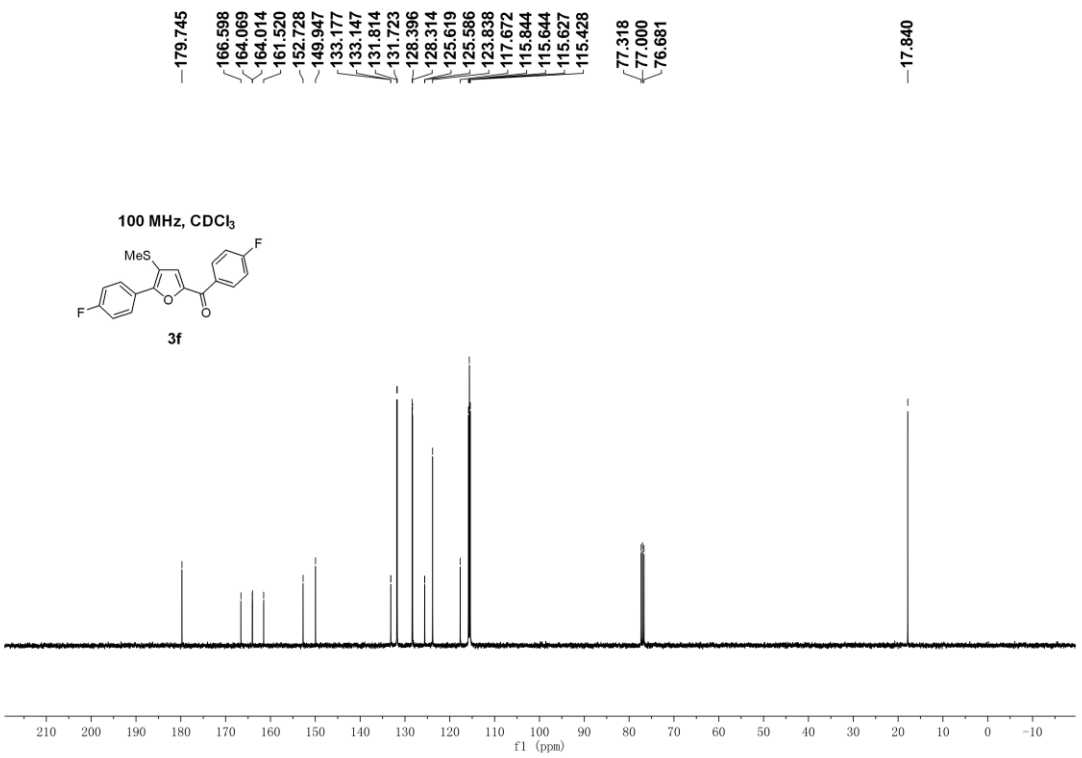
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128.314
125.619
125.586
123.838
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115.644
115.627
115.428
77.318
77.000
76.681
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100 MHz, CDCl3
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F
F
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3f
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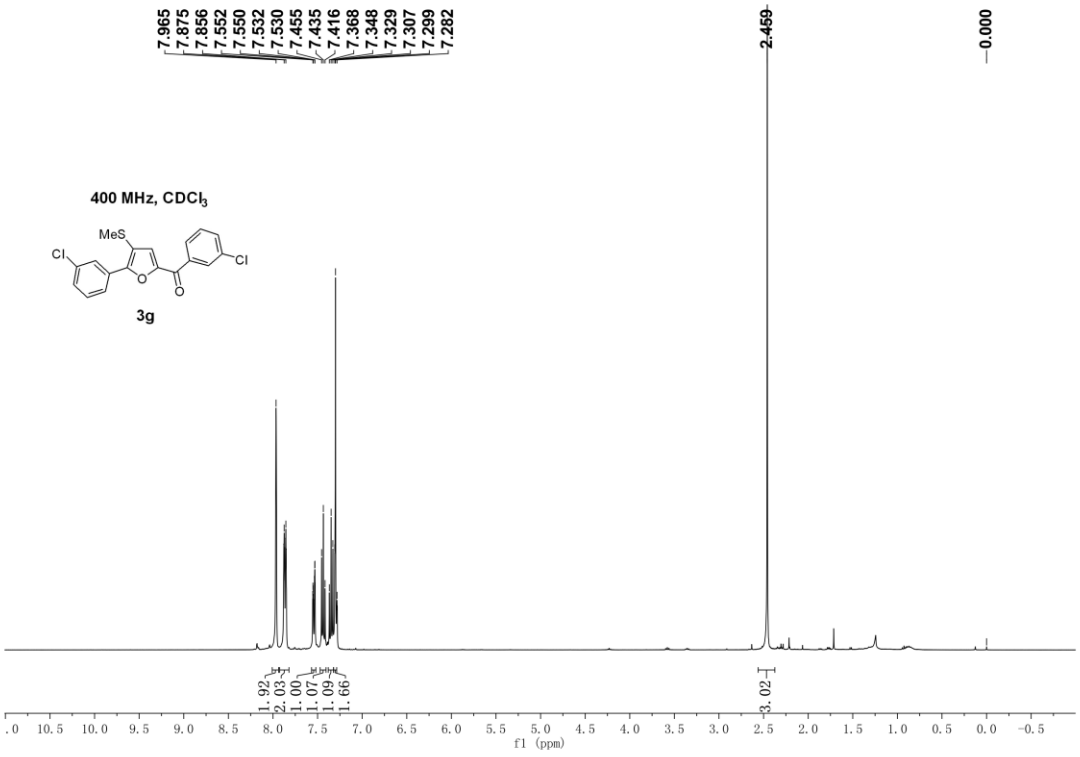
f1 (ppm)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400 MHz, CDCl3
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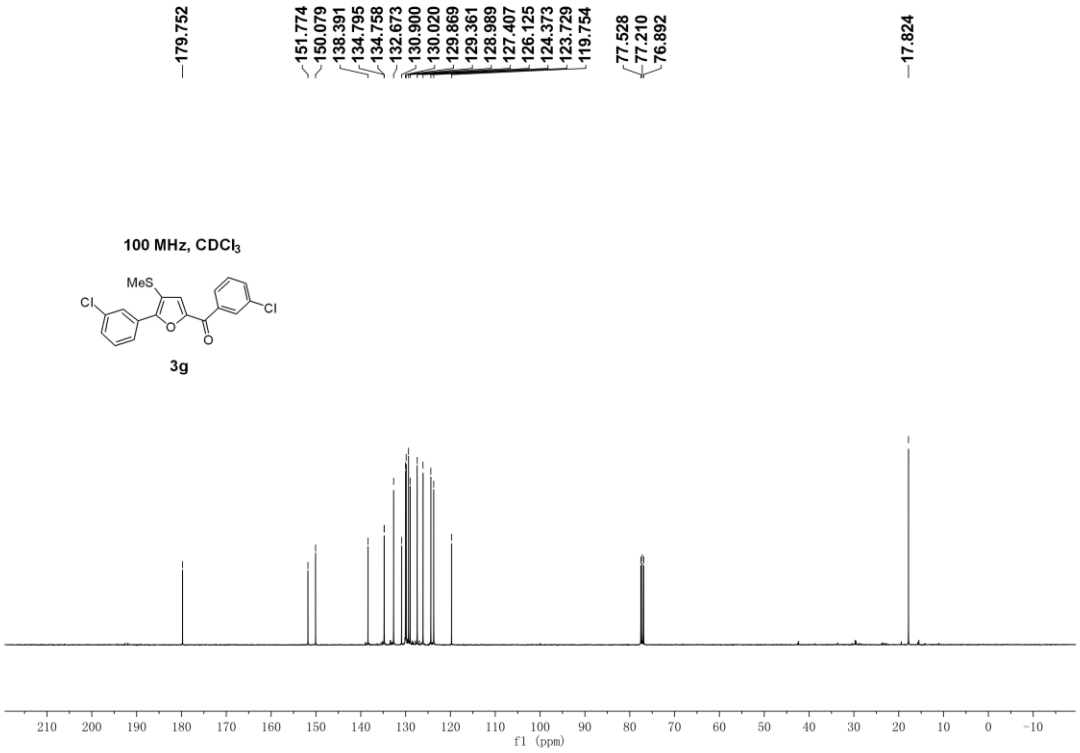
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Cl
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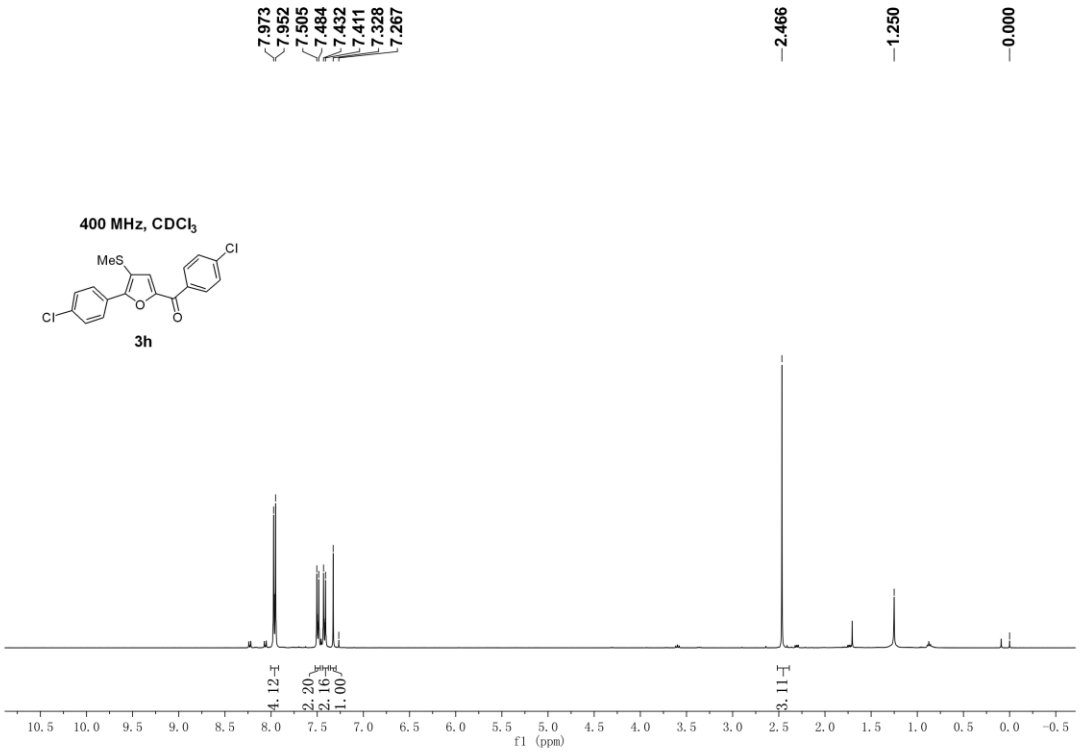
O
3g
f1 (ppm)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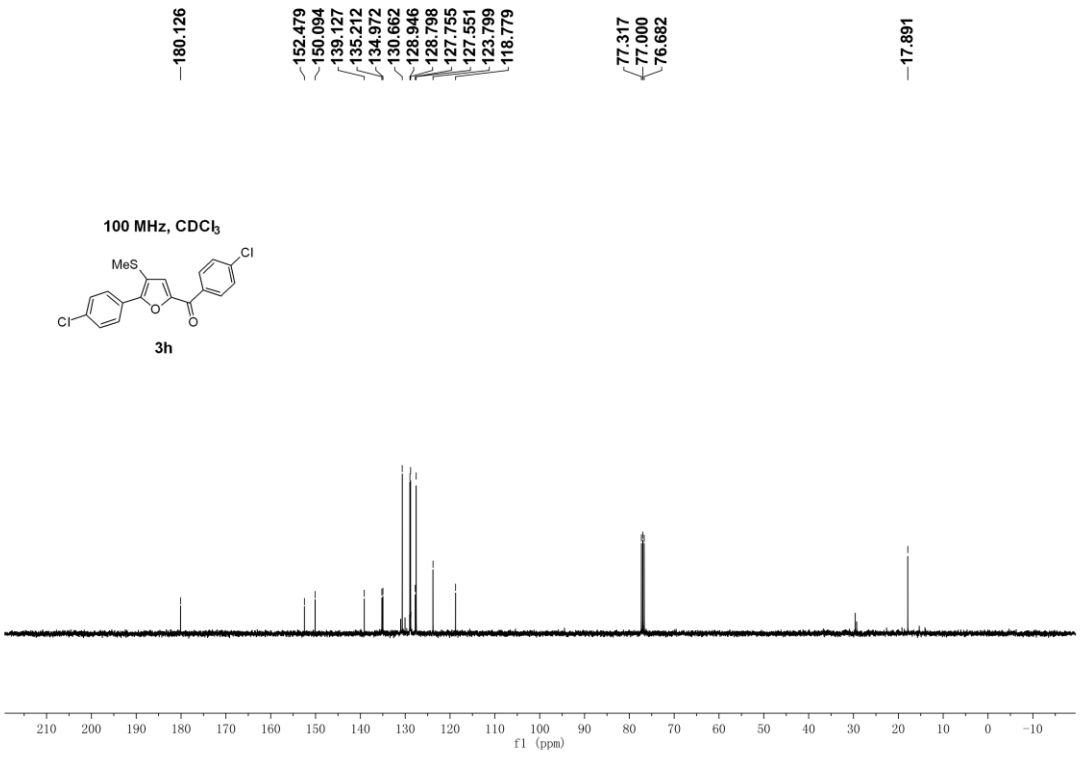
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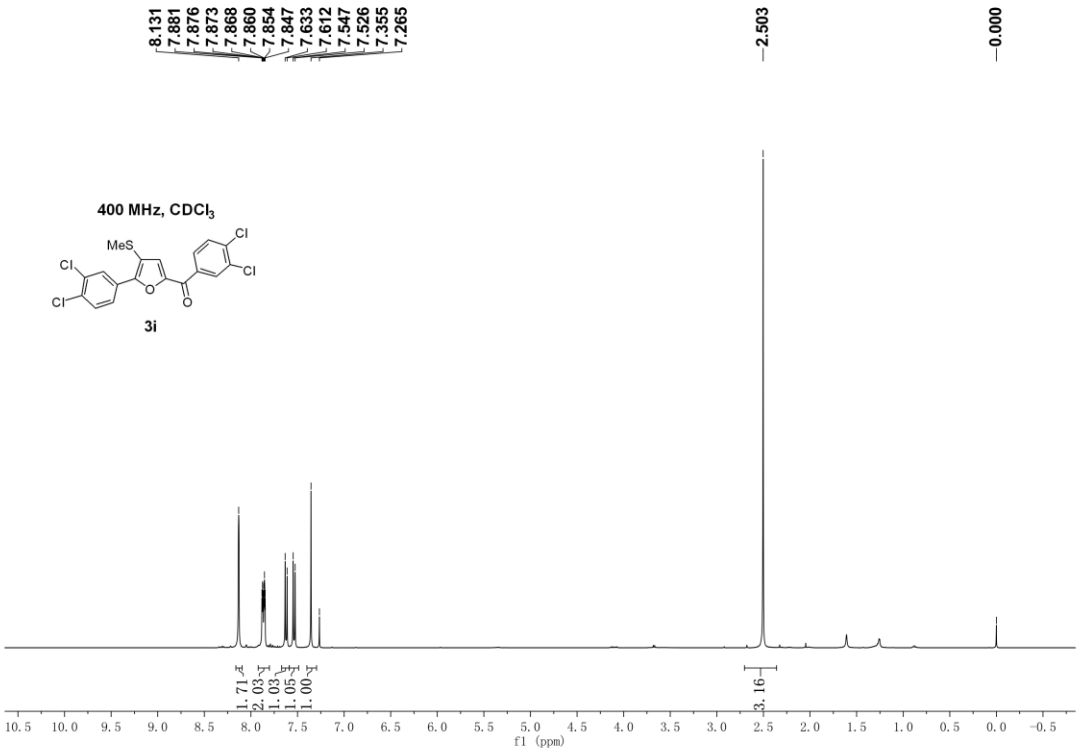
O
3h
f1 (ppm)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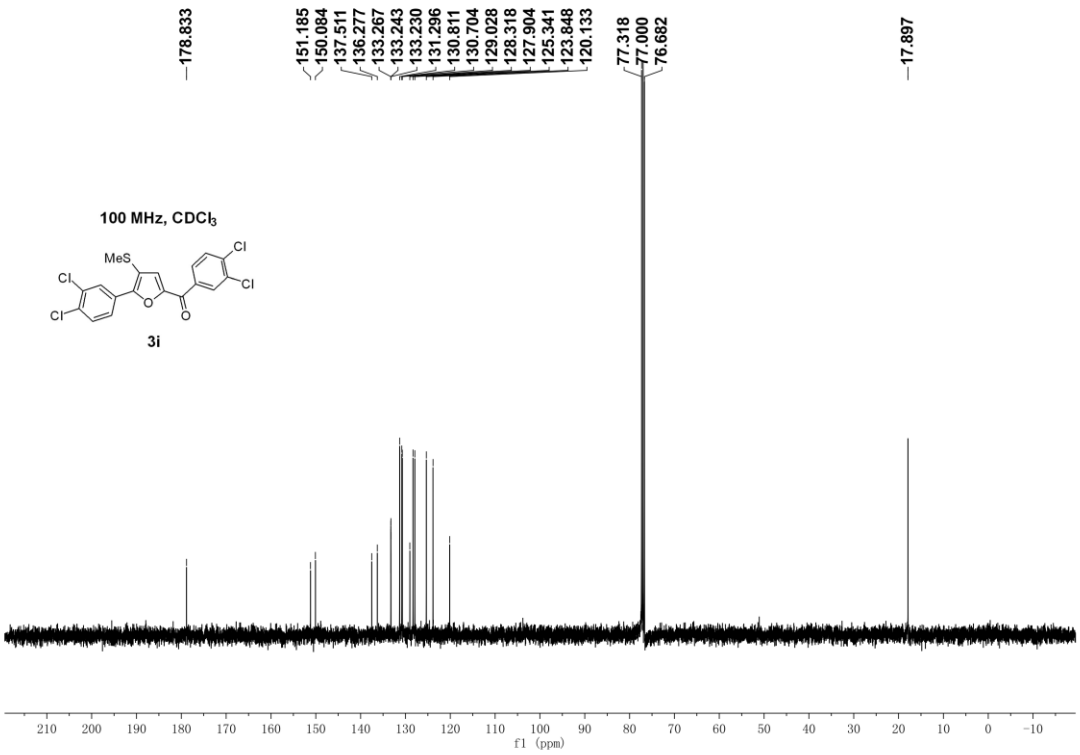
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127.904
125.341
123.848
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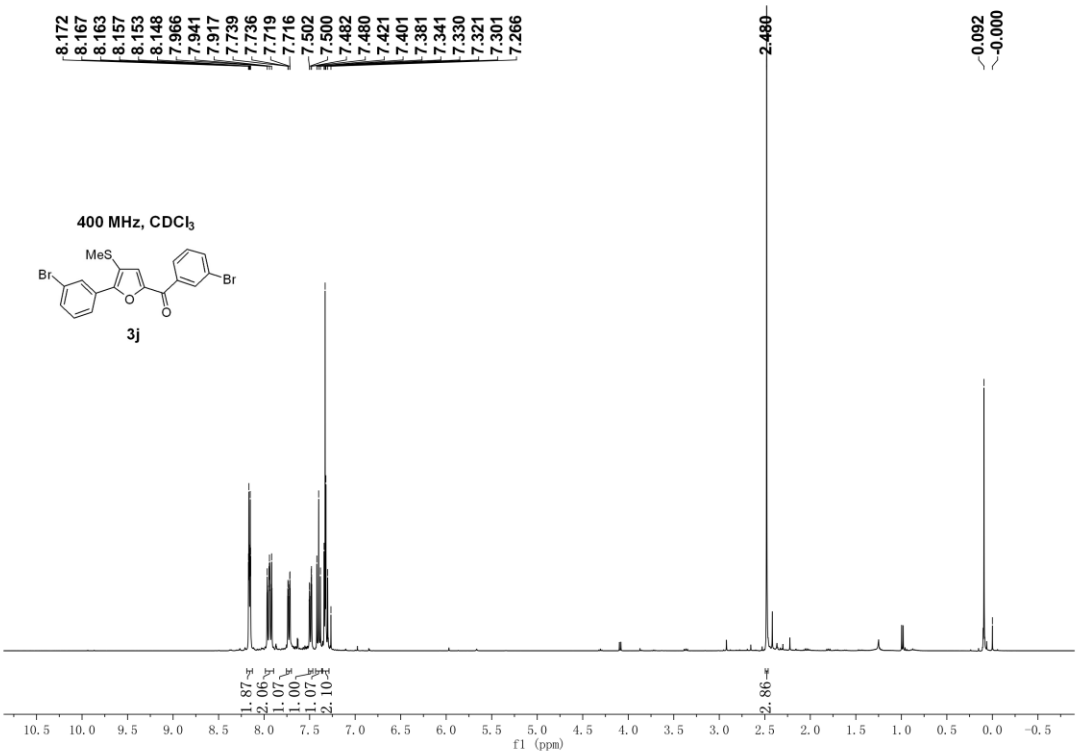
3i
f1 (ppm)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Br
O
O
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1.07
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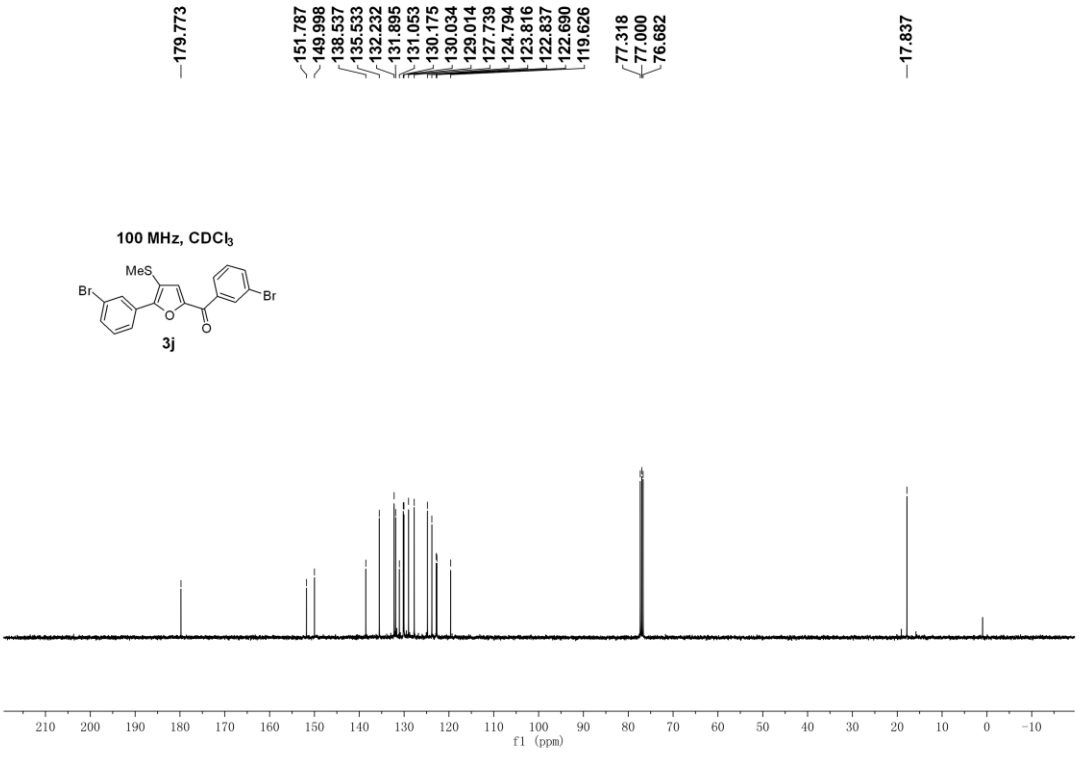
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119.626
77.318
77.000
76.682
17.837
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Br
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O
3j
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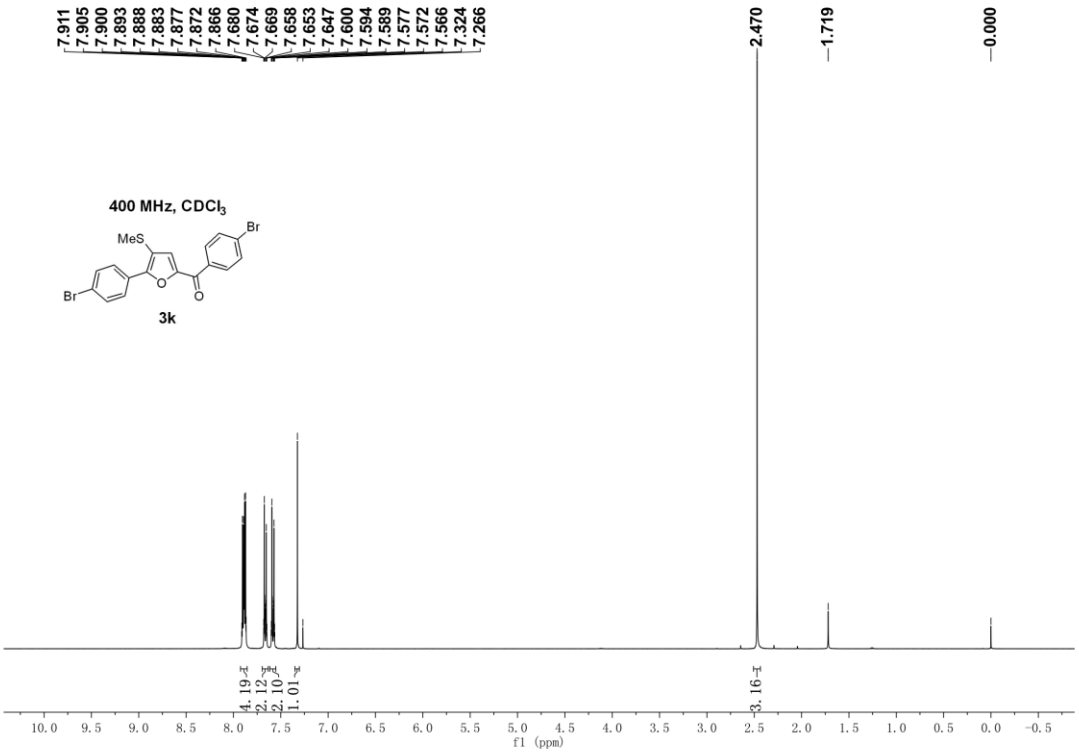
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7.572
7.566
7.324
7.266
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Br
O
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3k
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2.12
2.10
1.01
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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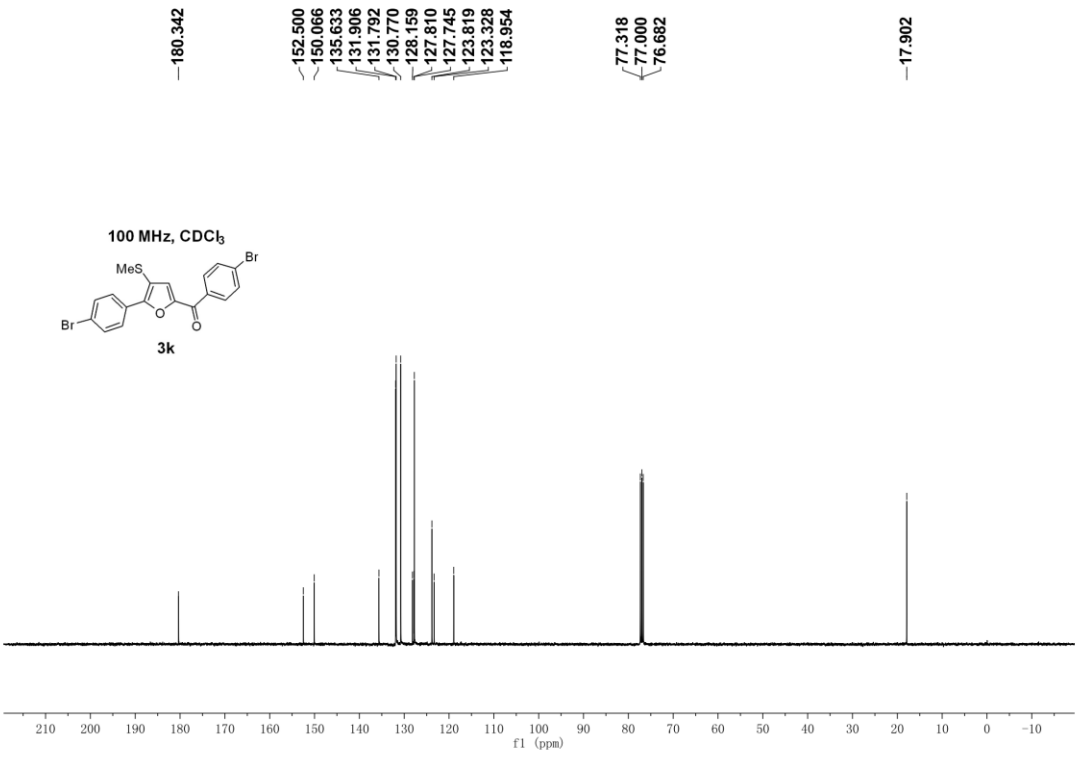
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77.000
76.682
17.902
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Br
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3k
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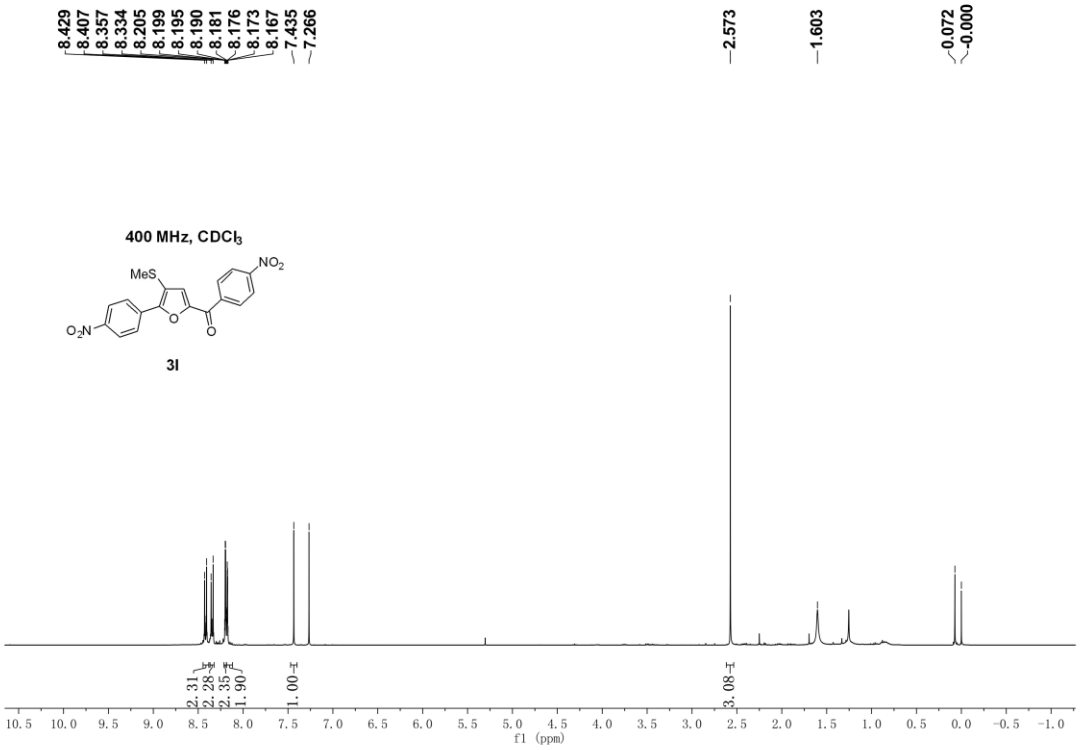
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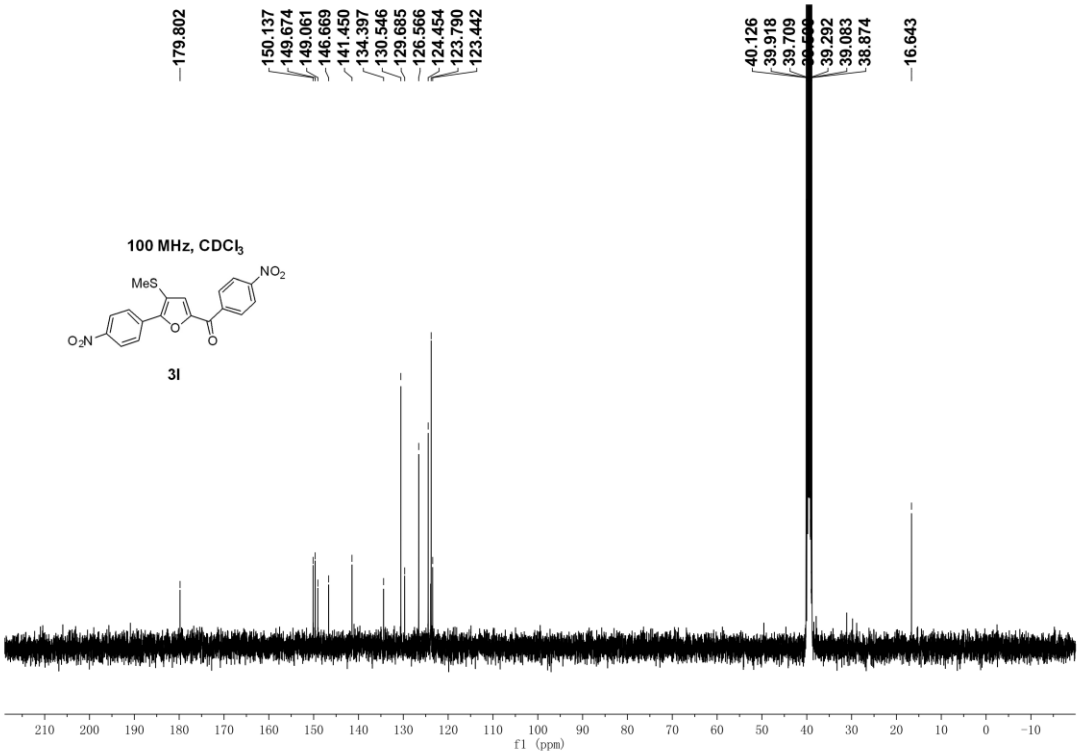
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100 MHz, CDCl3
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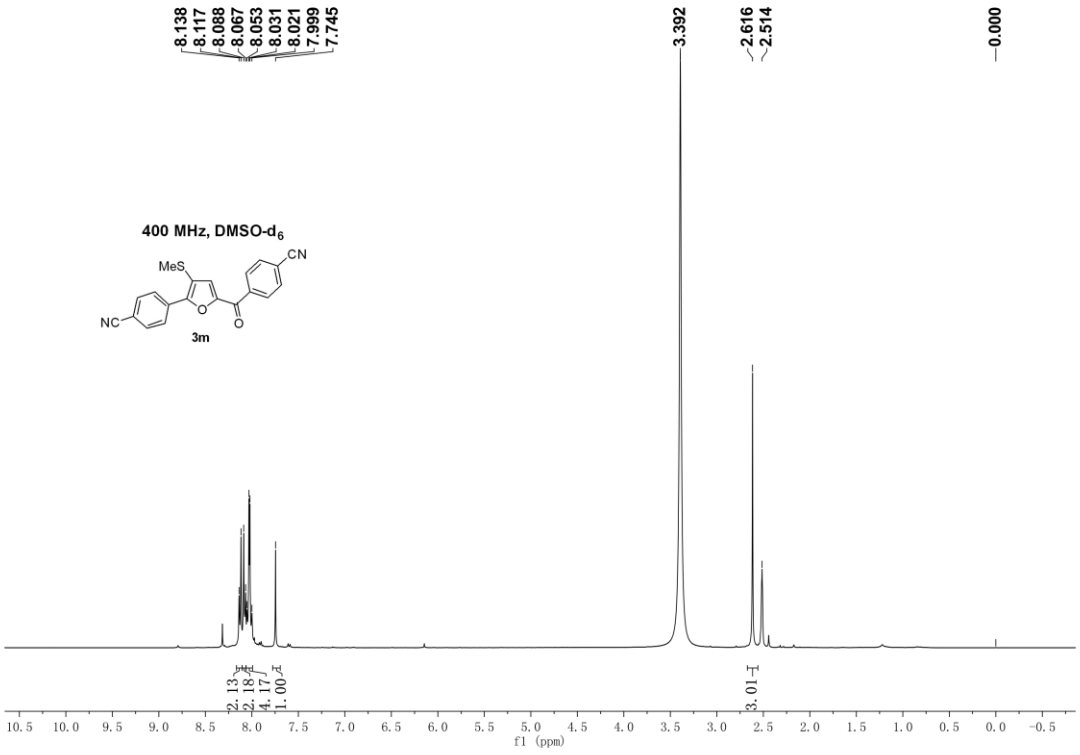
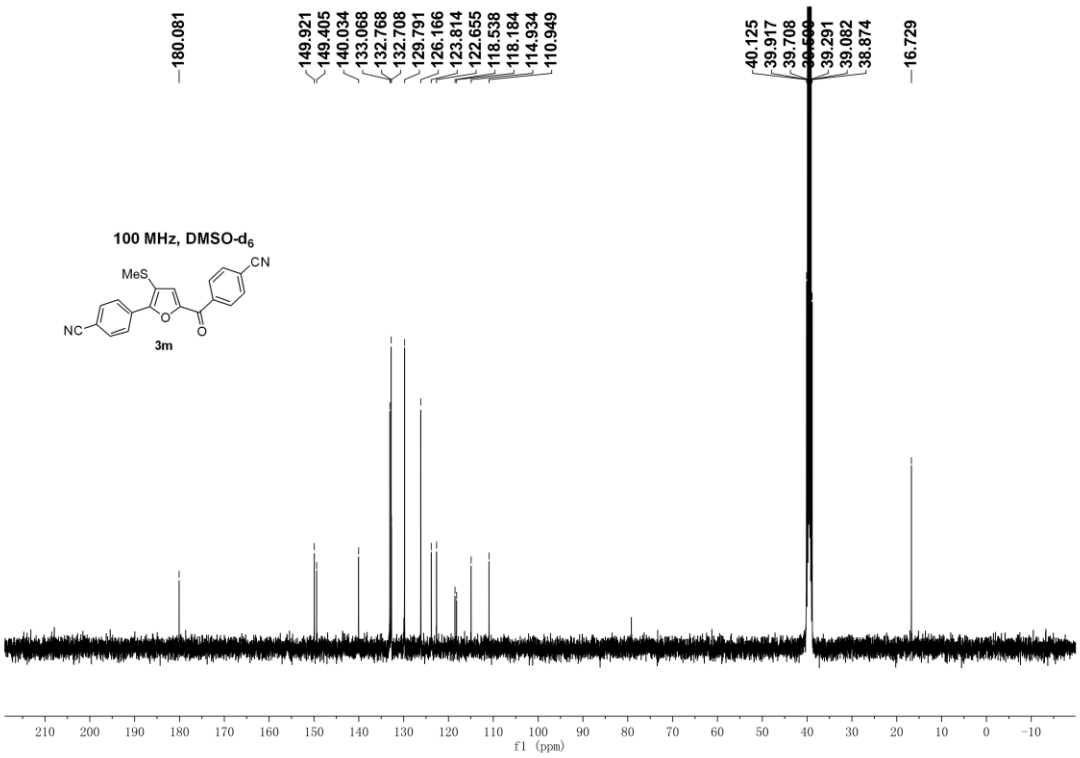
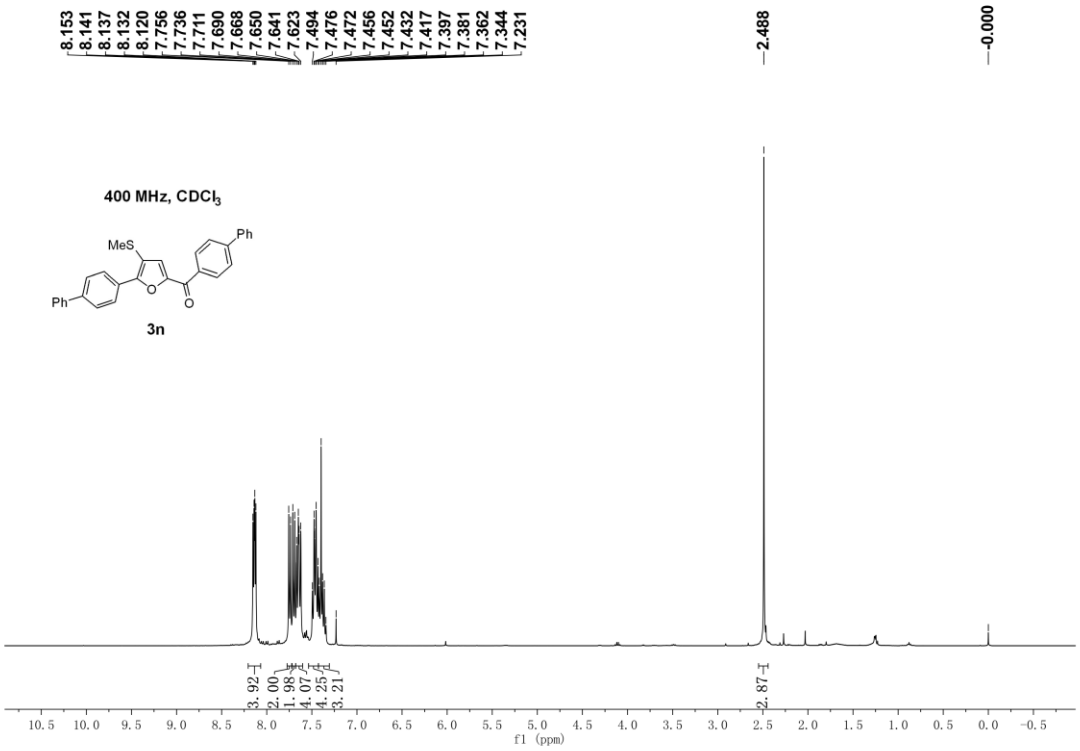
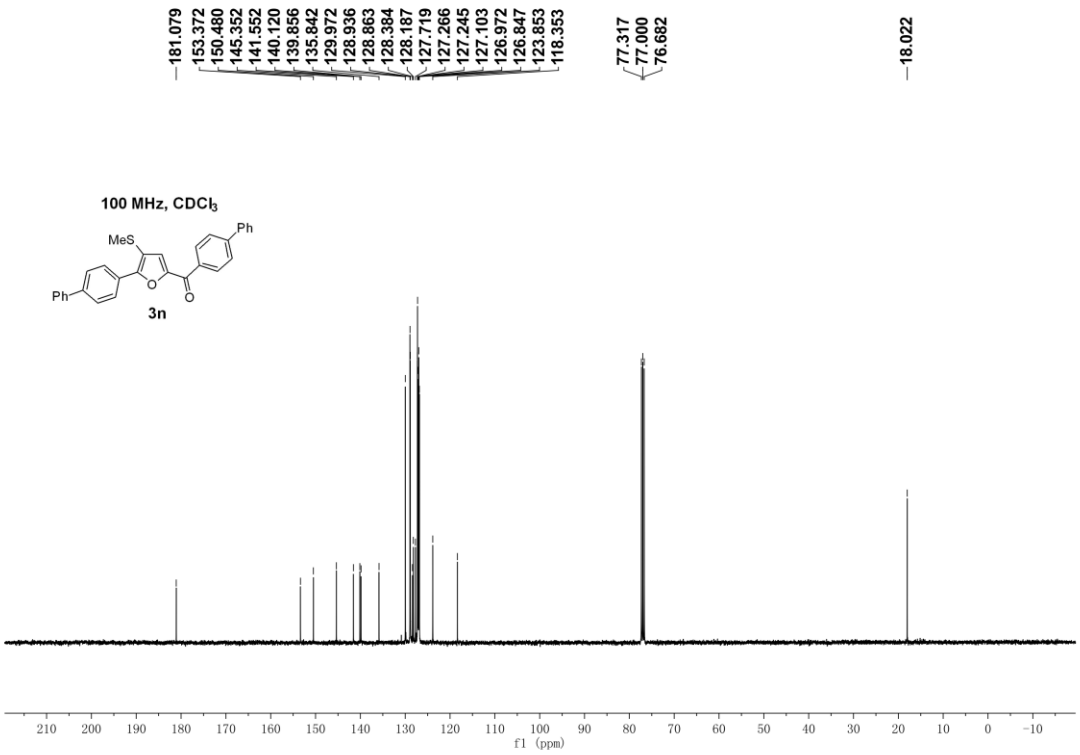
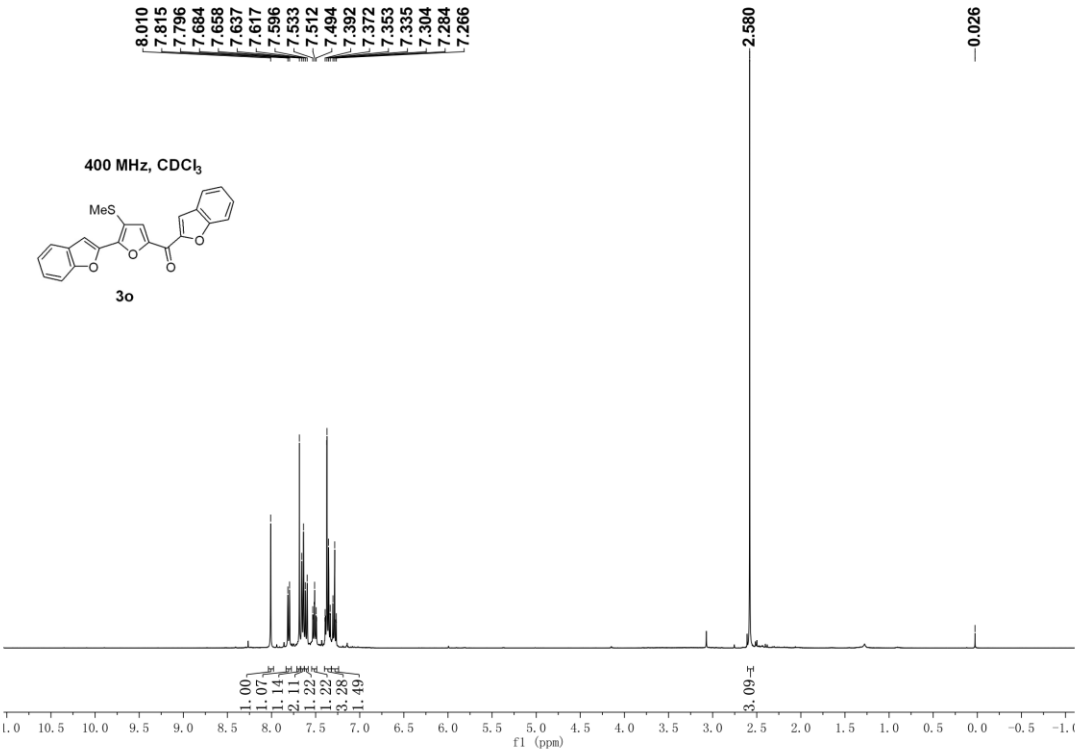
NO2
O2N
O
O
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

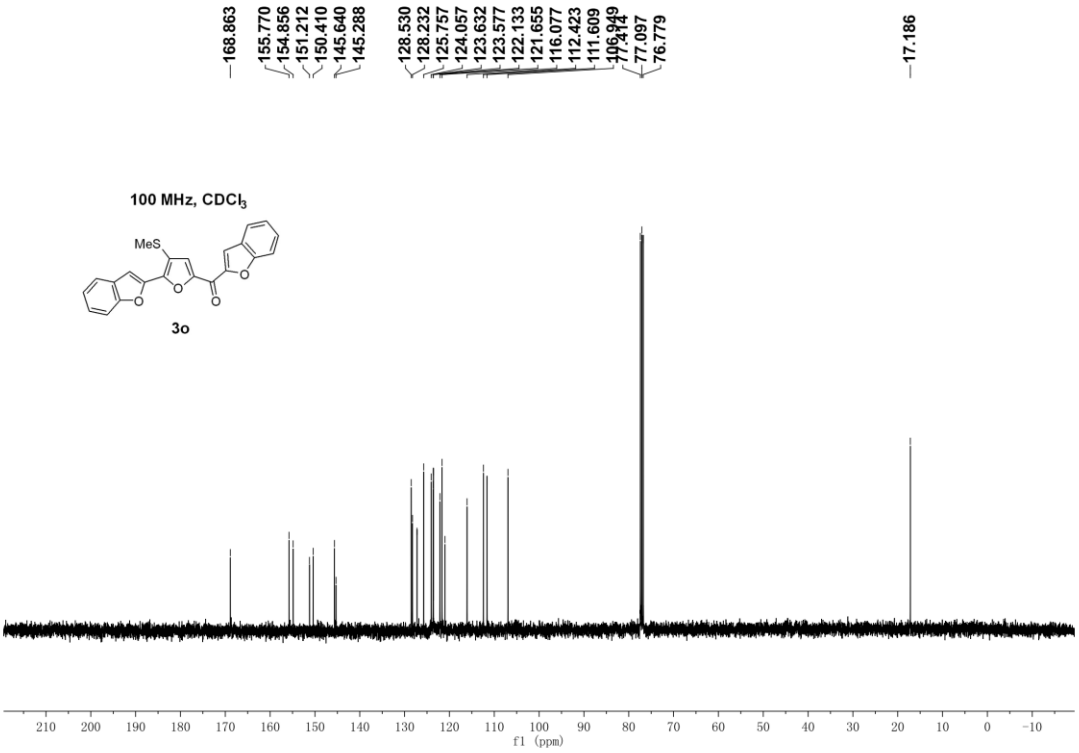

8.138
8.117
8.088
8.067
8.053
8.031
8.021
7.999
7.745
3.392
2.616
2.514
0.000
400 MHz, DMSO-d6
MeS
CN
NC
O
O
3m
2.13
2.18
4.17
1.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

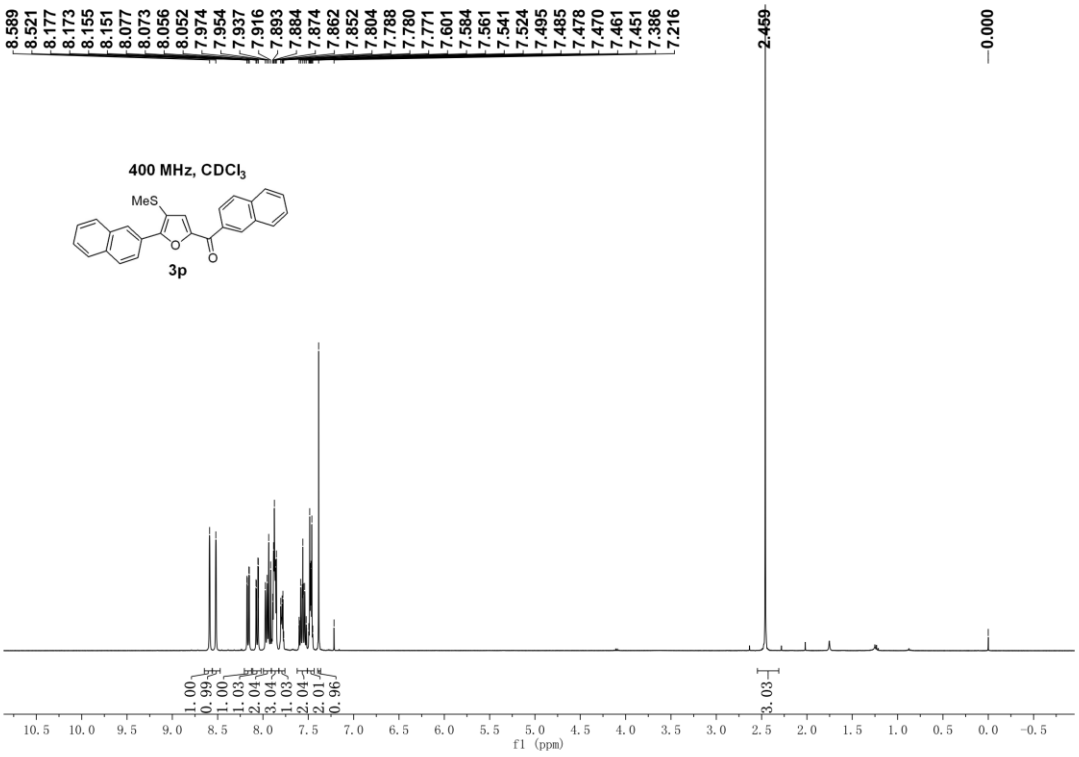

180.081
149.921
149.405
140.034
133.068
132.768
132.708
129.791
126.166
123.814
122.655
118.538
118.184
114.934
110.949
40.125
39.917
39.708
39.500
39.291
39.082
38.874
16.729
100 MHz, DMSO-d6
MeS
CN
NC
O
O
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

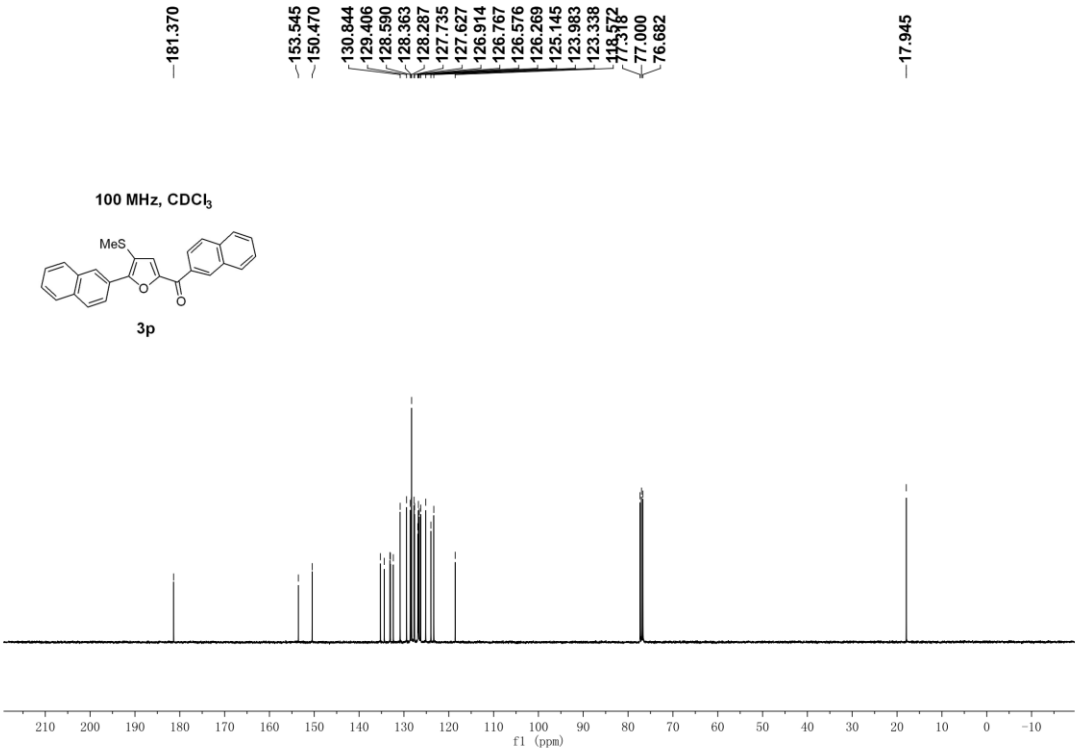

8.153
8.141
8.137
8.132
8.120
7.756
7.736
7.711
7.690
7.668
7.650
7.641
7.623
7.494
7.476
7.472
7.456
7.452
7.432
7.417
7.397
7.381
7.362
7.344
7.231
2.488
-0.000
400 MHz, CDCl3
MeS
Ph
Ph
O
O
3n
3.92
2.00
1.98
4.07
4.25
3.21
2.87
f1 (ppm)

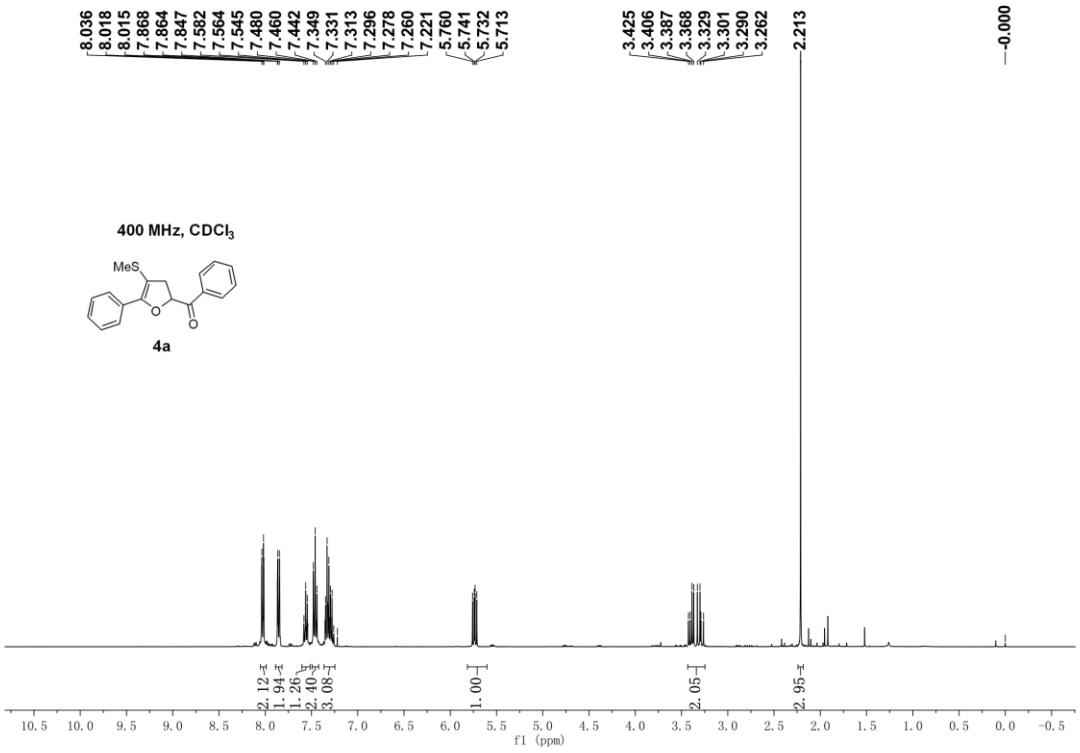

181.079
153.372
150.480
145.352
141.552
140.120
139.856
135.842
129.972
128.936
128.863
128.384
128.187
127.719
127.266
127.245
127.103
126.972
126.847
123.853
118.353
77.317
77.000
76.682
18.022
100 MHz, CDCl3
MeS
Ph
Ph
O
O
3n
f1 (ppm)

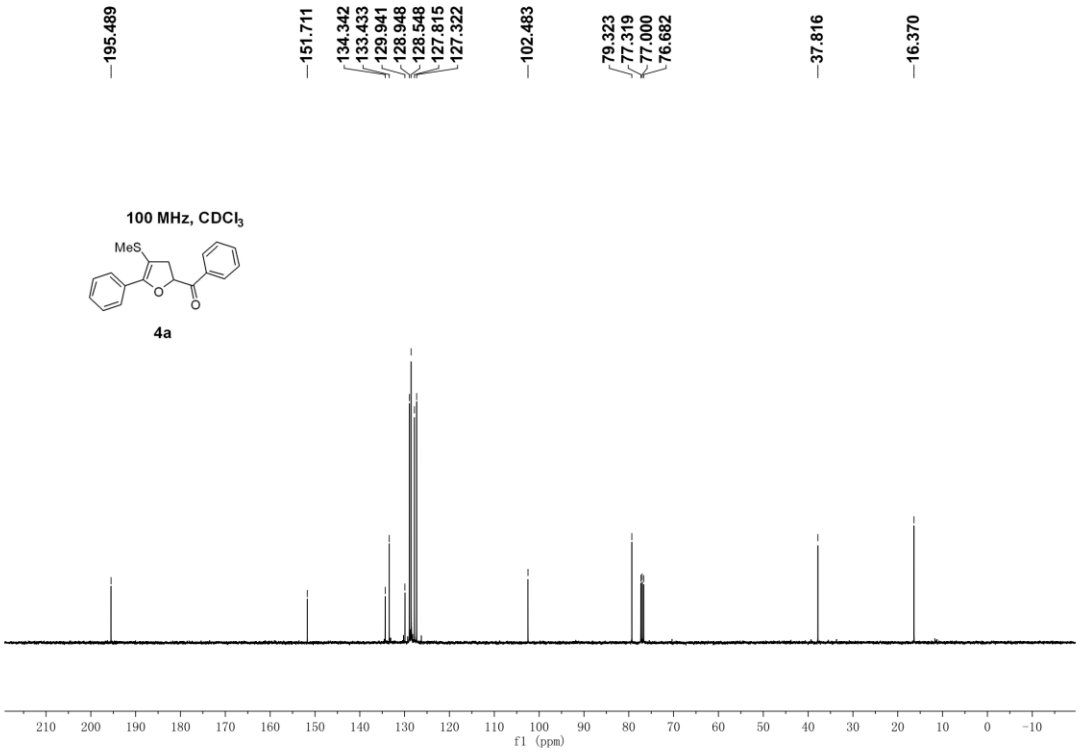

8.010
7.815
7.796
7.684
7.658
7.637
7.617
7.596
7.533
7.512
7.494
7.392
7.372
7.353
7.335
7.304
7.284
7.266
2.580
0.026
400 MHz, CDCl3
MeS
3o
1.00
1.07
1.14
2.11
1.22
1.22
3.28
1.49
3.09
f1 (ppm)


168.863
155.770
154.856
151.212
150.410
145.640
145.288
128.530
128.232
125.757
124.057
123.632
123.577
122.133
121.655
116.077
112.423
111.609
106.949
77.414
77.097
76.779
17.186
100 MHz, CDCl3
MeS
3o
f1 (ppm)


8.589
8.521
8.177
8.173
8.155
8.151
8.077
8.073
8.056
8.052
7.974
7.954
7.937
7.916
7.893
7.884
7.874
7.862
7.852
7.804
7.788
7.780
7.771
7.601
7.584
7.561
7.541
7.524
7.495
7.485
7.478
7.470
7.461
7.451
7.386
7.216
2.459
0.000
400 MHz, CDCl3
MeS
O
O
3p
1.00
0.99
1.00
1.03
2.04
3.04
1.03
2.04
2.01
0.96
3.03
f1 (ppm)


181.370
153.545
150.470
130.844
129.406
128.590
128.363
128.287
127.735
127.627
126.914
126.767
126.576
126.269
125.145
123.983
123.338
118.572
77.318
77.000
76.682
17.945
100 MHz, CDCl3
MeS
O
O
3p
f1 (ppm)


8.036
8.018
8.015
7.868
7.864
7.847
7.582
7.564
7.545
7.480
7.460
7.442
7.349
7.331
7.313
7.296
7.278
7.260
7.221
5.760
5.741
5.732
5.713
3.425
3.406
3.387
3.368
3.329
3.301
3.290
3.262
2.213
0.000
400 MHz, CDCl3
MeS
O
O
4a
2.12
1.94
1.26
2.40
3.08
1.00
2.05
2.95
f1 (ppm)


195.489
151.711
134.342
133.433
129.941
128.948
128.548
127.815
127.322
102.483
79.323
77.319
77.000
76.682
37.816
16.370
100 MHz, CDCl3
MeS
O
O
4a
f1 (ppm)